

Number of Gaussian primitives in the basis.

These supplementary functions are only used in the calculation of vibrational (IR) modes.

```

1      TOTAL NUMBER OF ATOM TYPES
6 6    ELECTRONIC AND NUCLEAR CHARGE
ALL    ALL-ELECTRON ATOM TYPE
1      NUMBER OF ATOMS OF TYPE CAR
ALL-CAR001
EXTRABASIS  CONTROLS USAGE OF SUPPLEMENTARY BASIS FUNCTIONS
12     NUMBER OF BARE GAUSSIANS
5 4 3   NUMBER OF S.P.D FUNCTIONS
0 0 1   SUPPLEMENTARY S.P.D FUNCTIONS:
  
```

Total number of basis functions of each type is sum of this column.

This example:
 $5+0 = 5$ s fxns.
 $4+0 = 4$ p fxns.
 $3+1 = 4$ d fxns.

Gaussian exponents

$\alpha_1 \alpha_2 \alpha_3$
 $\alpha_4 \alpha_5 \alpha_6$
 Etc.

Contraction coefficients for 1st basis fxn.

$C^1_1 C^1_2 C^1_3$
 $C^1_4 C^1_5 C^1_6$
 Etc.

Contraction coefficients for 2nd basis fxn.

$C^2_1 C^2_2 C^2_3$
 $C^2_4 C^2_5 C^2_6$
 Etc.

5 s fxns.

Diffuse s fxns.

Diffuse p fxns.

4 p fxns.

```

22213361D+05 .33317370D+04 .75790135D+03
21454372D+03 .69924889D+02 .25086135D+02
95910418D+01 .38024557D+01 .14891854D+01
57487653D+00 .21494732D+00 .77209650D-01
  
```

```

.19792249D+00 .36998977D+00 .63644615D+00
.10124931D+01 .14480787D+01 .17173689D+01
.14931932D+01 .68987161D+00 .86072247D-01
-.16566695D-02 .37766033D-03 -.47105343D-04
  
```

```

-.45005260D-01 -.84621052D-01 -.14496564D+00
-.23535601D+00 -.34215368D+00 -.44595124D+00
-.45263971D+00 -.32216414D+00 -.12988420D-01
.20135471D+00 .12769912D+00 .14135467D-01
  
```

```

.00000000D+00 .00000000D+00 .00000000D+00
.00000000D+00 .00000000D+00 .00000000D+00
.00000000D+00 .00000000D+00 .00000000D+00
.10000000D+01 .00000000D+00 .00000000D+00
  
```

```

.00000000D+00 .00000000D+00 .00000000D+00
.00000000D+00 .00000000D+00 .00000000D+00
.00000000D+00 .00000000D+00 .00000000D+00
.00000000D+00 .10000000D+01 .00000000D+00
  
```

```

.00000000D+00 .00000000D+00 .00000000D+00
.00000000D+00 .00000000D+00 .00000000D+00
.00000000D+00 .00000000D+00 .00000000D+00
.00000000D+00 .00000000D+00 .10000000D+01
  
```

```

.23138630D-01 .42649133D-01 .74658851D-01
.12024115D+00 .18351176D+00 .24706804D+00
.30714219D+00 .31372706D+00 .26726340D+00
.14756585D+00 .47585576D-01 .72796459D-02
  
```

```

.00000000D+00 .00000000D+00 .00000000D+00
.00000000D+00 .00000000D+00 .00000000D+00
.00000000D+00 .00000000D+00 .00000000D+00
.10000000D+01 .00000000D+00 .00000000D+00
  
```

```

.00000000D+00 .00000000D+00 .00000000D+00
.00000000D+00 .00000000D+00 .00000000D+00
.00000000D+00 .00000000D+00 .00000000D+00
.00000000D+00 .10000000D+01 .00000000D+00
  
```

```

.00000000D+00 .00000000D+00 .00000000D+00
.00000000D+00 .00000000D+00 .00000000D+00
.00000000D+00 .00000000D+00 .00000000D+00
.00000000D+00 .00000000D+00 .10000000D+01
  
```

Diagram illustrating the basis functions for the 120 vibrational modes of a molecule, showing the distribution of basis functions across different categories.

The basis functions are categorized into four groups, each represented by a 6x6 block in the matrix:

- Diffuse d fxns.** (Top-left block, 6x6)
- 4 d fxns.** (Top-right block, 6x6)
- Only included in basis in vibrational mode** (Bottom-right block, 6x6)
- Other basis functions** (Bottom-left block, 6x6)

The matrix is labeled **ELECTRONS WFOUT**.

4 d fxns.

Only included in basis in vibrational mode

ELECTRONS
WFOUT

$$\phi_N(\vec{x}) = \sum_{p=1}^{n_p} C_p^N |\vec{x}|^l Y_{lm}(\hat{x}) e^{-\alpha_p |\vec{x}|^2}$$

In practice a symmetric molecular orbital is the actual basis used in the calculations formed from linear combinations of the above.